



Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment Program

Barbara Helland
Advanced Scientific Computing Research
Barbara.Helland@science.doe.gov

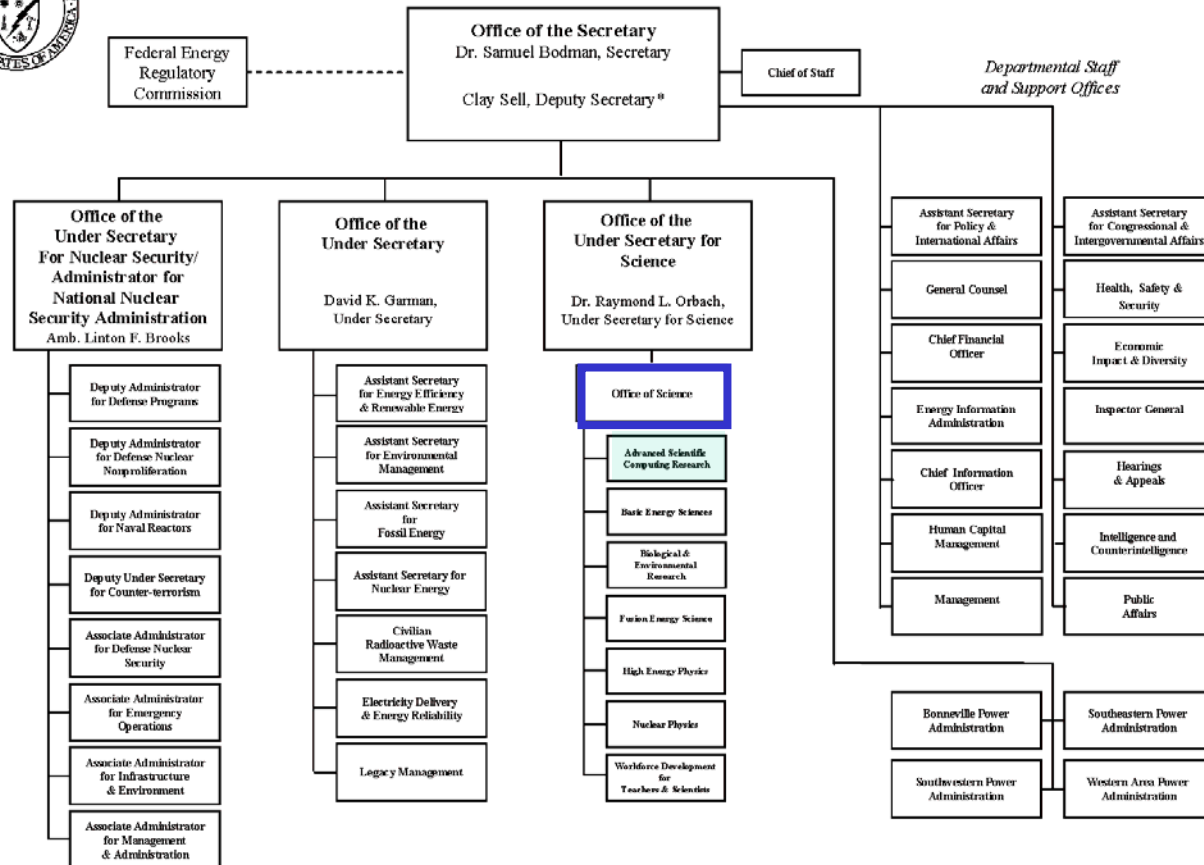


Department of Energy Organizational Structure

Advanced Scientific Computing Research Program



DEPARTMENT OF ENERGY



* The Deputy Secretary also serves as the Chief Operating Officer

26 Oct 06

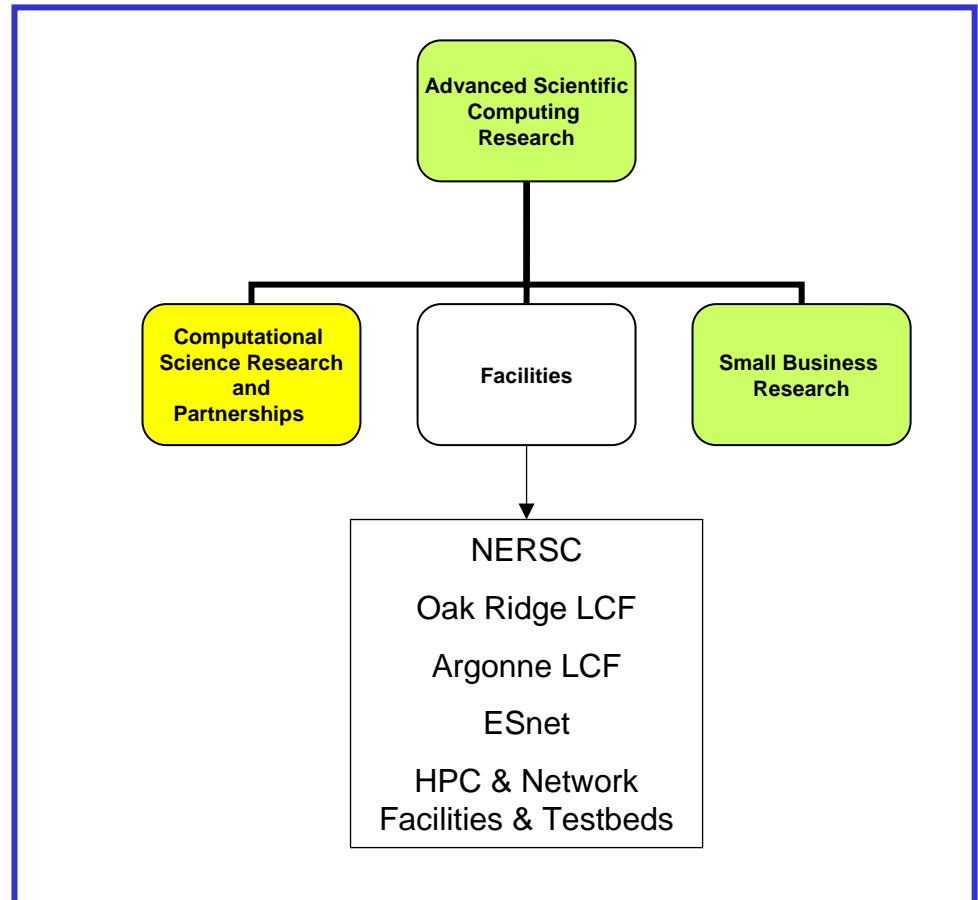


Advanced Scientific Computing Research

Advanced Scientific Computing Research Program

ASCR Mission: Steward of DOE's Computational Science, Applied Mathematics, Computer Science, High-Performance Computing and Networking Research for open science. Deploy and operate high performance computing user facilities at LBNL, ANL, and ORNL

ASCR Vision: Best in class advancing science and technological innovation through modeling and simulation



<http://www.science.doe.gov/ascr>



ASCR High Performance Computing Resources

Advanced Scientific Computing Research Program

- **High Performance Production Computing Facility (NERSC)**
 - Delivers high-end capacity computing to entire DOE SC research community
 - Large number of projects (200 – 300)
 - Medium- to very-large-scale projects that occasionally need a very high capability
 - Annual allocations
- **Leadership Computing Facilities**
 - Delivers highest computational capability to national and international researchers through peer-reviewed Innovative and Novel Computational Impact on Theory and Computation program
 - Small number of projects (10 – 20)
 - Multiple year allocations

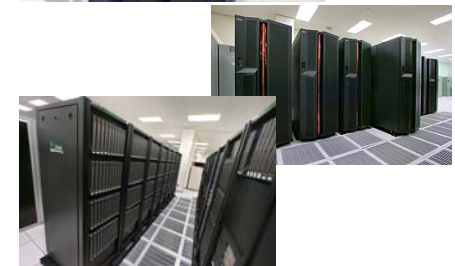


Current Facilities

Advanced Scientific Computing Research Program

- **NERSC**

- 10 Teraflop IBM SP 375 RS/6000 (Seaborg) with 6080 processors, 7.2 terabytes aggregate memory
- 6.7 Teraflop IBM Power 5 (Bassi) with 888 processors, 3.5 terabytes aggregate memory
- 3.1 Teraflop LinuxNetworkx Opteron cluster (Jacquard) with 712 processors, 2.1 terabytes aggregate memory



- **LCF at Oak Ridge**

- 119 teraflop Cray XT3/XT4 (Jaguar) with 11,708 dual core AMD Opteron processor nodes, 46 terabytes aggregate memory
- 18.5 Teraflop Cray X1E (Phoenix) with 1,024 multi-streaming vector processors,



- **Argonne LCF**

- 5.7 Teraflop IBM Blue Gene/L (BGL) with 2,048 PPC processors





Future Facility Upgrades

Advanced Scientific Computing Research Program

- ALCF
 - 100 teraflop IBM Blue Gene/P delivered by end of 2007
 - 250-500 teraflop upgrade to IBM Blue Gene/P in late 2008
- LCF – Oak Ridge
 - Cray XT4 upgraded to 250 TF by end of 2007
 - 1 Petaflop Cray Baker system to be delivered by end of 2008
- NERSC
 - 100+ teraflop Cray XT4 in operation by October 2007





Innovative and Novel Computational Impact on Theory and Experiment- INCITE

Advanced Scientific Computing Research Program

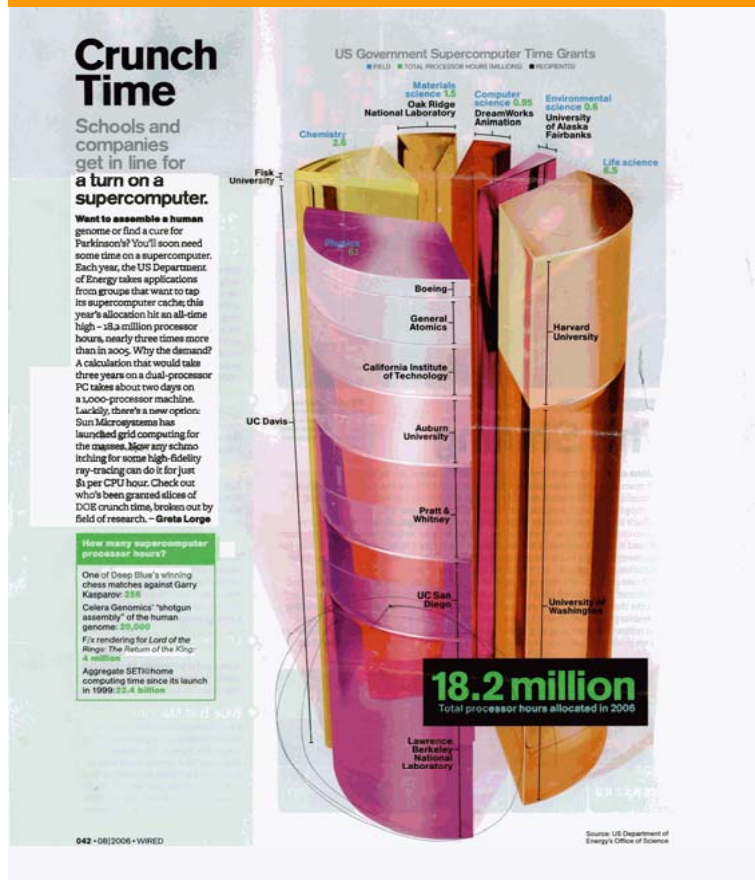
- Initiated in 2004
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer and computational readiness reviewed
- 2004 Awards: 4.9 Million processor hours at NERSC awarded to three projects
- 2005 Awards: 6.5 Million processor hours at NERSC awarded to three projects



INCITE 2006

Advanced Scientific Computing Research Program

Wired Magazine, August, 2006, pg. 42

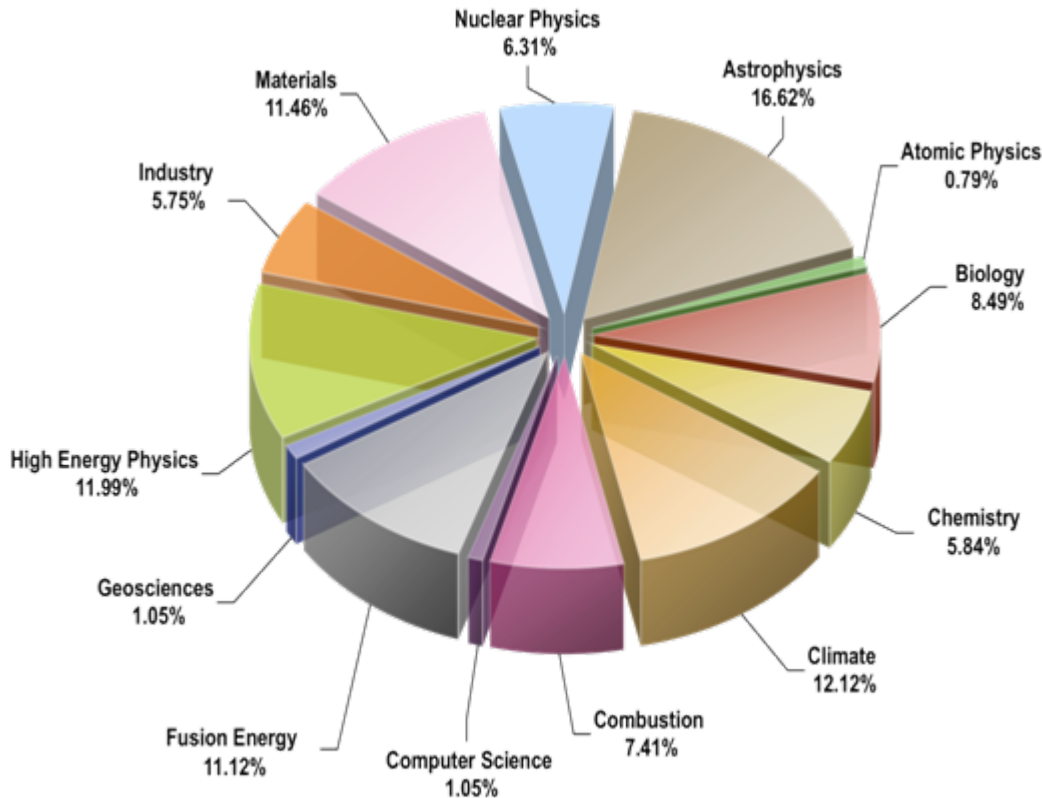


- Expanded to include SC high end computing resources at PNNL, ORNL and ANL in addition to LBNL and multiple year requests.
- Received 43 proposals requesting over 95 million processor hours.
 - 60% from Universities
 - 40% had funding from other federal research agencies
- 15 Awards for over 18.2 million processor hours



2007 INCITE Allocations by Disciplines

Advanced Scientific Computing Research Program



- 80% of Leadership Computing Facilities allocated through INCITE
- 88 new proposals and 20 renewal proposals received requesting over 250 Million processor hours
- 95 Million processor hours allocate to 45 projects (26 new proposals and 19 renewal)



2008 INCITE

Advanced Scientific Computing Research Program

New 2008 INCITE Call for Proposals for over **0.25 Billion** processor hours

2008 INCITE Call for Proposals

For the fifth consecutive year, DOE's Office of Science is inviting proposals from scientists and engineers for the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. The INCITE program will award significant allocations on some of the world's most powerful supercomputers to innovative, large-scale computational science projects to enable high-impact advances. Scientists from the national and international research community will be able to request allocations on machines at Oak Ridge National Laboratory (ORNL), Lawrence Berkeley National Laboratory (LBNL), Pacific Northwest National Laboratory (PNNL) and Argonne National Laboratory (ANL).

In 2008 the Office of Science expects to award up to a quarter of a billion hours through the INCITE program. Specifically, 80% of the leadership-class Cray computers at ORNL and the IBM Blue Gene resources at ANL are allocated through the INCITE program. In addition to the leadership-class resources at ORNL and ANL, 10% of the National Energy Research Scientific Computing Center (NERSC) high-performance computing resources at LBNL and 5% of the Hewlett-Packard MPP system at PNNL will be made available to INCITE. A full description of the resources available under this call can be [found here](#).

The INCITE program is open to all scientific researchers and research organizations, including industry. The program seeks computationally intensive research projects of large scale, with no requirement of current Department of Energy sponsorship, that can make high-impact scientific advances through the use of a large allocation of computer time, resources, and data storage. Proposals can be for one to three years in length. A small number of large awards, including possible renewals of current multi-year allocations, is anticipated. The INCITE program also provides opportunities for industry to use DOE high-end computing resources as encouraged in reports and case studies by the Council on Competitiveness. For more information on previous awards, see <http://www.science.doe.gov/ascr/incite/INCITEPreviousAwards.html>.

Successful proposals will describe high-impact scientific research in terms suitable for peer review in the area of research and also be appropriate for general scientific review comparing them with proposals in other disciplines. Applicants must also present evidence that they can make effective use of a major fraction of the processors of the high performance computing systems offered for allocation. Applicant codes must demonstrate readiness to run on the requested computing system(s).

Eligibility: This program specifically encourages proposals from universities, other research institutions and industry. Industry is specifically solicited to propose challenging problems that may be solved using high performance computing. Current sponsorship by the Office of Science of the Department of Energy is not a requirement for this program.

Proposers who wish to engage in scientific research of their own or in collaboration with investigators at the four National Laboratories with the intent to publish meaningful results in open peer-reviewed literature ("non-proprietary users") are eligible. Those Proposers who wish the maximum protection for their own proprietary data loaded onto the DOE computers and/or who wish to keep the results of their computations proprietary ("proprietary users") are also eligible under the special requirements set forth below.

- Deadline 11:59 pm EDT August 8, 2007
- <http://hpc.science.doe.gov>